

# Frequently asked questions

## General

### More details

### More information

For more information, refer to the [user manual](#).

## Developers

Morpheus is developed by Jörn Starruß and [Walter de Back](#) at the [IMC group](#) headed by prof. [Andreas Deutsch](#).

We are part of the [Center for High Performance Computing](#) at the [Technische Universität Dresden](#), Germany.

## Modeling

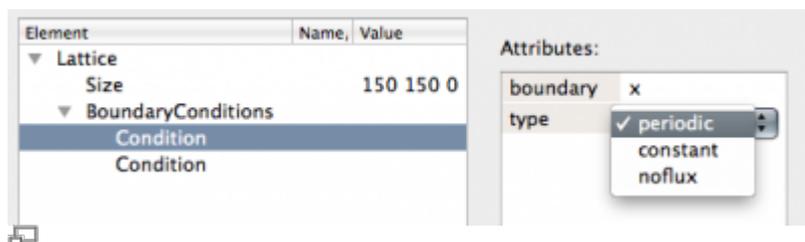
### Boundary conditions

#### Types of Boundary Conditions

Morpheus provides three types of boundary conditions.

| Types of BoundaryConditions |             |  |
|-----------------------------|-------------|--|
| Name                        | Synonym     | Meaning  |
| <b>Periodic</b>             | Wrap-around | Border states are mapped to states at opposite border. |
| <b>Constant</b>             | Dirichlet   | Border states have specified constant values.          |
| <b>Noflux</b>               | Neumann     | Derivative at border is zero.                          |

These can be specified in Space → Lattice → BoundaryConditions. These define the **structure** of the boundaries.



The structure of the borders is defined in Space → Lattice → BoundaryConditions.

Note that there are six boundaries ( $x$ ,  $-x$ ,  $y$ ,  $-y$ ,  $z$ ,  $-z$ ). All need to be specified, except when

periodic boundaries are used (in which case  $x=-x$ ,  $y=-y$ ,  $z=-z$ ).

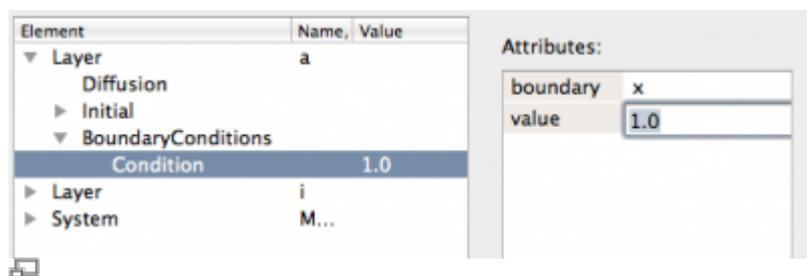
### Constant boundary condition

To define constant boundaries, select constant in Space → Lattice → BoundaryConditions.

To specify the **values** the constant boundaries should take, we distinguish between reaction-diffusion models (PDE) and cell-based models.

### Reaction-diffusion models (PDE)

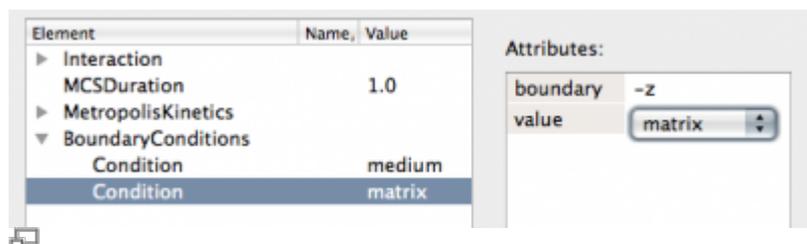
When using constant boundary conditions, values used at the boundary of a reaction-diffusion model can be specified in PDE → Layer → BoundaryConditions. Assuming nonzero diffusion, this causes a constant influx (or efflux) from (at) that boundary. The default value is \$0.0\$.



Specify values at boundaries in PDE → Layer → BoundaryConditions.

### Cell-based models

A particular medium cell type can be specified at constant boundaries. First, define a cell type of type medium under CellTypes. To specify this at the boundary of a cell-based model with constant boundary conditions, use CPM → BoundaryConditions.



Specify cell types at boundary in CPM → BoundaryConditions.

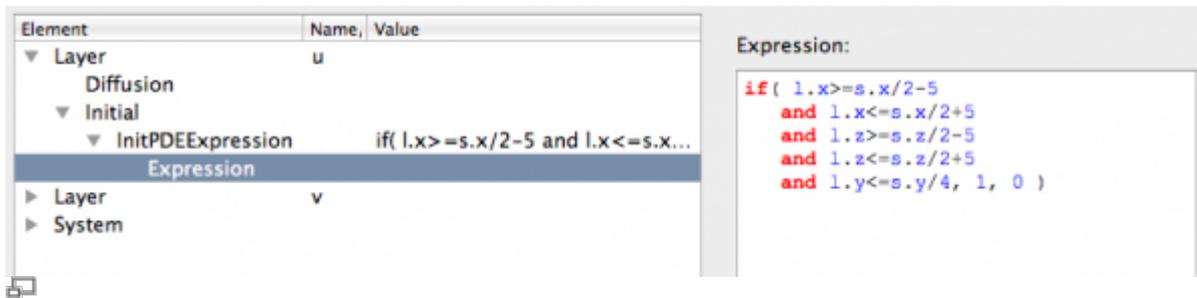
### Initial conditions

To specify initial conditions, we distinguish between reaction-diffusion models (PDE) and cell-based models.

### Reaction-diffusion models (PDE)

To set an initial condition for a species in the reaction-diffusion model, specify it in PDE → Layer → Initial → InitPDEExpression → Expression.

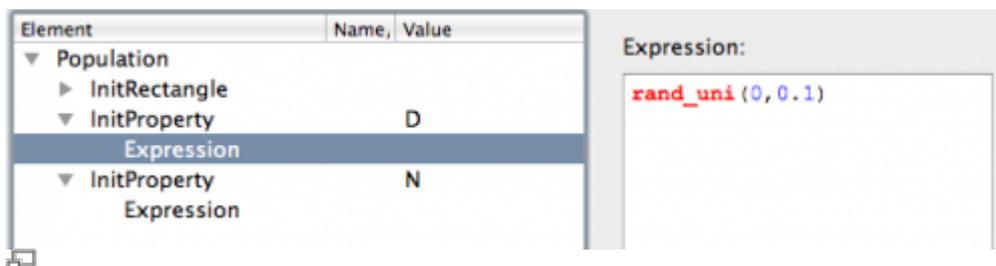
Note that you can express the initial condition in terms of the lattice size using the symbols set in Space → Lattice → Size/symbol (here: s) and Space → SpaceSymbol (here: l).



Set initial conditions of PDE using InitPDEExpression in terms of spatial symbols for lattice size.

## Cell-based models

Initial conditions for a Property of a CellType are specified when you define the Population of cells. Set the initial values using CellPopulations → Population → InitProperty.



Set initial condition for cell Properties using InitProperty in the Population definition.

## Random seed

### Random seed

- Mersenne Twister from C\+\+ compiler (gcc version > 4.6) or Boost library when available.
- Time → RandomSeed

### Reproducibility

- In simulation using multithreading (openMP), each thread gets its own random seed. Therefore, to reproduce exact results, one needs to specify the same random seed as well as the same number of threads.

## Time scales

Specifying time scales is important, especially in multiscale models in which dynamics occur at multiple temporal scales.

In Morpheus, we distinguish three time scales:

1. Global time: defines the time frame of a simulation.
2. Monte Carlo time scale: defines updating scheme of cells.
3. System time scale: defines updating and dynamics of systems of (differential) equations.

### Global time

Each model must specify a **global time** scheme under Time that runs from StartTime to StopTime. All other processes are scheduled within this time frame.

For **dimensionless models**, a sensible choice for the global time scheme would be from 0 to 1. For an example, see the [cell cycle model](#) (File → Examples → MultiScale → CellCycle).

Alternatively, for **dimensional models**, time units can be specified (msec, sec, min, hours, days) such that one could define the global time to run from 20 hours to 7 days. Default interpretation is 1 sec.

### Monte Carlo time scale (CPM)

The time scale of cellular Potts models can be specified using `CPM → MCSDuration`. This defines the interval between Monte Carlo steps, in terms of global time scheme.

For example, if the global time is defined from 0 → 1, and `MCSDuration` is set unitless to  $1.0 \cdot 10^{-2}$ , a total of 100 Monte Carlo steps will be performed during the simulation.

Alternatively, if the global time is defined with dimensions from 0 hours to 1 hours, and `MCSDuration` is set to 1.0 sec, a total of 3600 Monte Carlo steps will be performed during the simulation.

Note that changing the `MCSDuration` time scale directly affects the CPM dynamics such as cell motility and cell shape changes. In fact, it will affect all processes under `CellTypes → CellType`, **except** the processes defined within `Systems`.

### System time scale (ODE/PDE)

To define the time scale for a System of (differential) equations, we need to distinguish between:

1. Numerical updating scheme: how often the equations with the systems are evaluated.
2. System dynamics: setting the time scale of ODE model dynamics, relative to the global time.

The numerical updating of a system of equations is defined in `System → time-step` (default=1), in terms of the global time scheme. This sets the accuracy of the numerical approximation (i.e. it is the  $\Delta t$  of the numerical solver), but does not affect the time scale of its dynamics.

To **change the time scale of the dynamics** of simulated ODE model, you can use the `System → time-scaling` attribute. This scales the rates of dynamics, while maintaining the accuracy (by automatically scaling the time-step). For an example, see the [multi-scale cell cycle model](#) (File → Examples → Multiscale → CellCycle).

## Spatial scale

### Lattice scale

- Space → `NodeLength`

This affects the diffusion coefficient in PDE models.

Dimensionless space is assumed, unless a unit is specified.

## Neighborhoods

### Types of Neighborhoods

Two types of neighborhood are used:

- Space → Lattice → Neighborhood: ...
- CPM → MetropolisKinetics → Neighborhood: ...

### Order and Distance

The number of neighboring nodes to include can be specified in two different units:

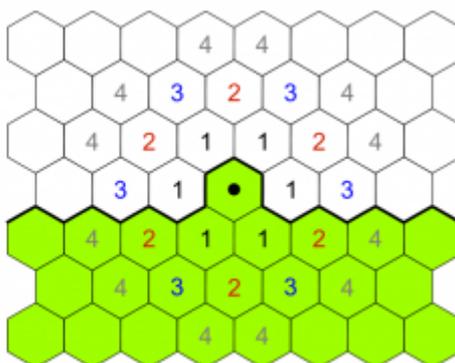
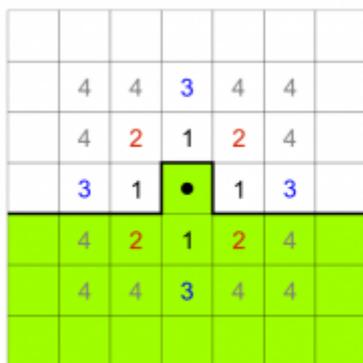
- Distance: All nodes  $\leq$  this distance are included in the neighborhood.
- Order: All nodes of this order are included in the neighborhood.

### Order

The "order" of a neighborhood is a measure of neighborhood size that expands in an alternating way axially and radially.

In a square lattice:

- Order 1: 4-member, axial (von Neumann)
- Order 2: 8-member, radial (Moore)
- Order 3: 12-member, axial
- ...



 Neighborhood orders 1-4 indicated by numbers around the focal node for a square and hexagonal lattice.

### "Function" or "Equation"?

Both are algebraic expressions, however:

- A Function defines a symbol, and it calculated whenever this symbol is used.
- An Equation changes the value of a symbol defined elsewhere (symbol - ref) and is calculated every time-step.  
 Note: if an Equation is part of a System, the time-step of the System overrules the one defined by the Equation itself.

|          | Attribute    | Evaluation   |
|----------|--------------|--|
| Function | symbol       | Evaluated when symbol is used  |
| Equation | symbol - ref | Evaluated every time - step (default=1), set result to referred Property |

## Analysis

### 2D Visualization (Gnuplot)

Use the Gnuplotter. See the [Examples](#) to learn how to use it.

### 3D Visualization (TIFF / VTK)

#### 3D visualization

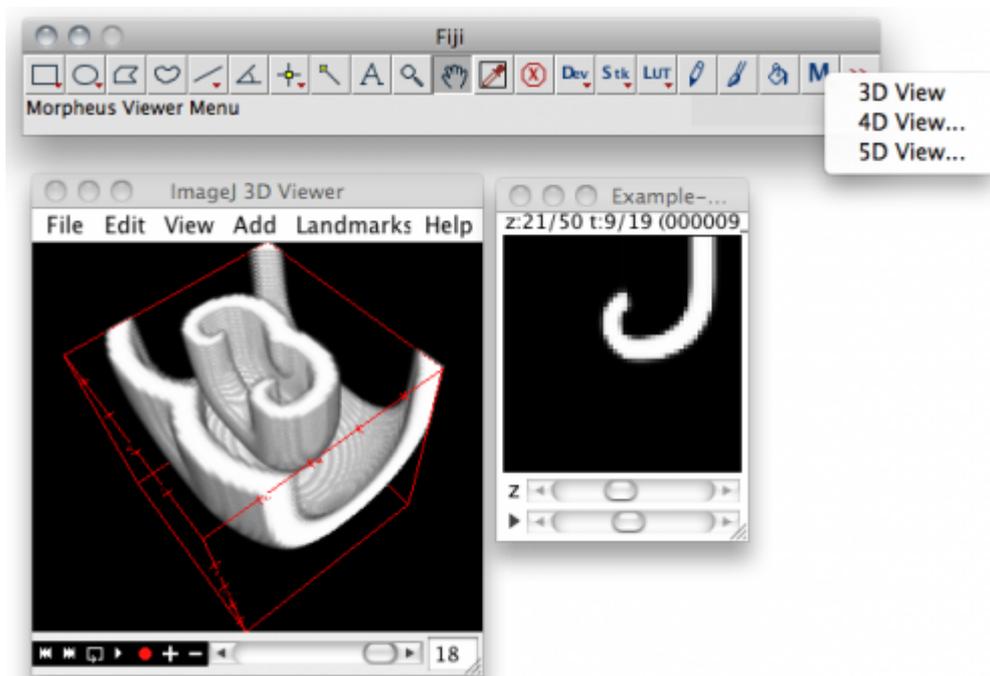
To visualize 3D simulations, Morpheus can write TIFF images stacks or VTK files.

These files can be rendered with external software, such as [Fiji](#) or [Paraview](#).

#### Viewing 3D TIFF images with Fiji/ImageJ

To export 3D images as TIFF z-stacks, use the Analysis → TiffPlotter plugin.

The resulting TIFF images can be opened using the 3D Viewer in [Fiji](#), an image processing package based on ImageJ (see Plugins → 3D Viewer).



Use TiffPlotter for 3D, 4D or 5D visualization in Fiji.

By concatenating TIFF stacks, you can also render 4D (3D+time) or even 5D (3D+time+channels) movies.

## Fiji Macros

We provide some simple Fiji macros to generate such 3D images and 4D/5D movies. To install them:

- Download [morpheus\\_fiji\\_viewers.zip](#)
- Extract contents in Fiji/macros
  - Mac: Select Applications/Fiji.app, then right-click and select Show Package Contents.
  - Ubuntu: Default location is \$HOME/Fiji.app/macros

This will install a new toolset in the Fiji interface called Morpheus Viewer from which the 3D/4D/5D viewers are available.

## Paraview

[Paraview](#) is an application for visualization of large 3D data sets in VTK format ([download here](#)).

## Data output and visualization

### Logger

*Note: this plugin will be restructured in the near future.*

The Logger periodically writes the values of the symbols specified in the Format to file.

Its Plot function can generate timeplots, or phase plots, depending on the columns selected for the axes. Note: these columns correspond to the column number in the generated data file (first column = 1).

### HistogramLogger

HistogramLogger calculates frequency distributions and writes them to file.

Its Plot function can generate timeplots.

## Parameter sweep / Batch processing

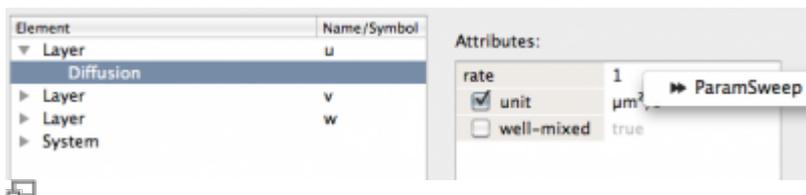
To explore the effect of a parameter on model behavior, you can set up a batch process called ParamSweep.

### 1. Select parameters

In the Attributes window, press right-click on a parameter and choose ParamSweep. A 'fast-forward' symbol appear indicating that this parameter is set for a parameter sweep.

Alternatively, if no Attributes windows is available (e.g. with Expression), right-click in the central window to select for ParamSweep.

Note that model parameters of any type can be explored (double, int, string, enum, etc.).



Right-click in Attributes window to select parameter for ParamSweep

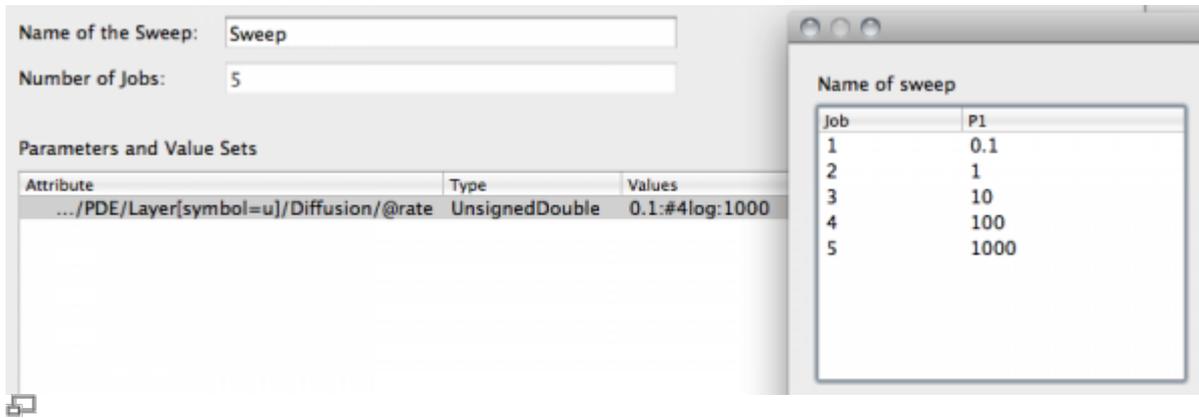
## 2. Set range of values

Once you have chosen a parameter, go to the ParamSweep view (see Documents window).

Here, you can specify a range of values for each parameter.

| Syntax                         | Example              | Generated sequence   | Description   |
|--------------------------------|----------------------|----------------------|---|
| <b>value1;value2;value3</b>    | 1.0;1.25;4           | 1.0;1.25;4           | Sequence of values  |
| <b>string1;string2;string3</b> | "square";"hexagonal" | "square";"hexagonal" | Sequence of strings                                       |
| <b>min:increment:max</b>       | 0:2:10               | 0;2;4;6;8;10         | Range of values with increment                            |
| <b>min:#steps:max</b>          | 0:#2:10              | 0;5;10               | Range of values with number of steps                      |
| <b>min:#steps[log]:max</b>     | 0.1:#2log:10         | 0.1;1.0;10.0         | Range of values with number of steps in logarithmic scale |

The Number of Jobs that will be generated is calculated and displayed.



Specify range of values in ParamSweep window and execute batch process by pressing Start.

## 3. Execute ParamSweep

To start a parameter sweep, **press Start in the toolbar** while you have the ParamSweep panel open.

Before it starts the batch process, Morpheus let's you check your jobs and parameters in a pop-up window.

Also note that batch processes can benefit from **parallel computing** by allowing multiple concurrent jobs, see Settings → Local → Concurrent Jobs.

Note that the parameter sweep is always run in Local mode (overrides Interactive mode).

## Multi-dimensional ParamSweeps

Multi-dimensional parameter sweep are generated by selecting multiple parameters for ParamSweep.

To couple multiple parameters such that they are incremented simultaneously, drag one over the other to 'pair' them.

### How to post-process results of a parameter sweep?

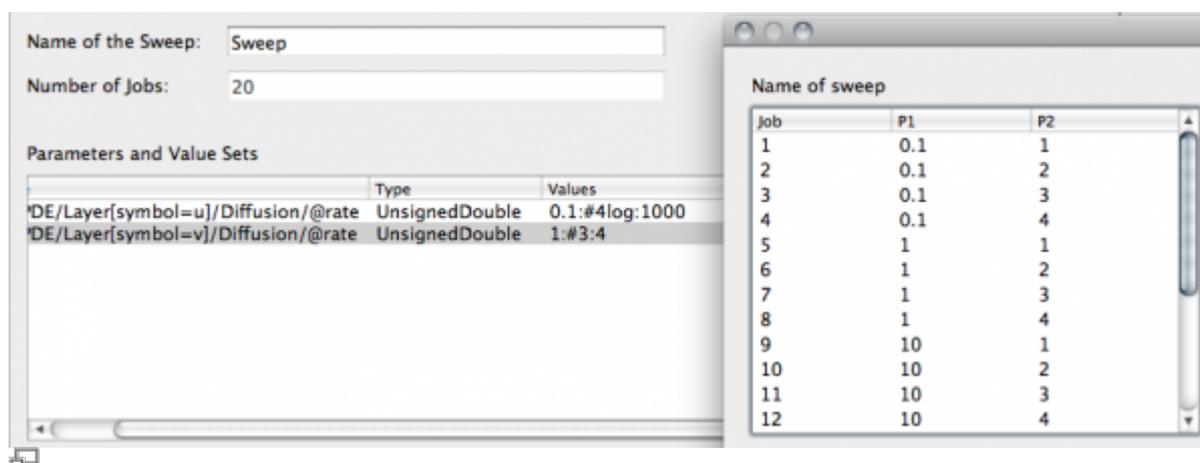
Morpheus does not include tools for post-processing of data. Thus, analyzing results should be done using your own favorite tools.

Yet, Morpheus does supply a few features that enable you to analyze results of parameter sweeps:

- Sweep summary: file containing data on parameters and the folder in which the results are saved.
- Python scripts:
  - morphMakeTable.py: generate  $\LaTeX$  table from images from a parameter sweep (using sweep summary)
  - morphSweepData.py: gather data from log files from a parameter sweep (using sweep summary)

### ImageTable

This option can be used to create a  $\LaTeX$  table of images from a parameter sweep. This is a simplified interface to the python script morphMakeTable.py.

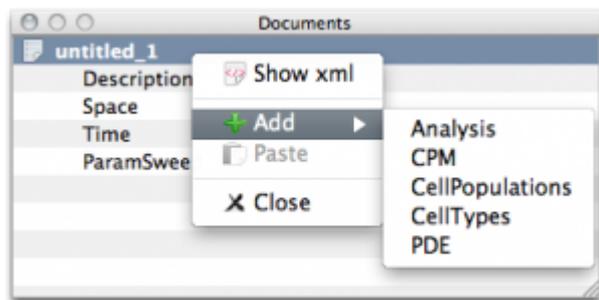


## Editing

### Add or remove model items

#### Add/Remove in Document view

To add or remove optional model components such as PDE, CellTypes, or CellPopulation, right-click in the Documents View and choose Add or Remove.

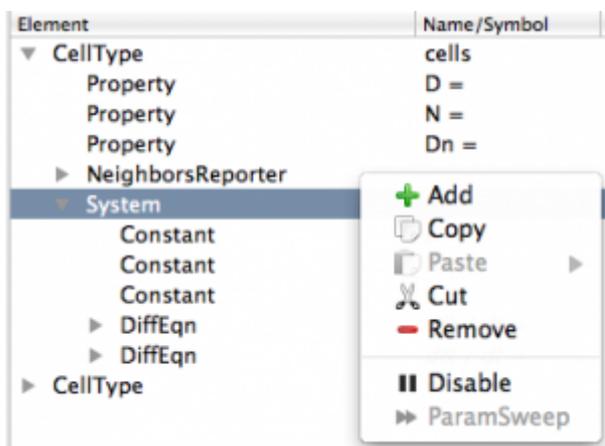


Right-click in the Documents view

### Add/Remove in Editor view

To add or remove optional plugins, right-click **on the parent node** and choose Add or Remove. The parent node is the place on which the new plugin should appear.

In case of Remove, you will be prompted to confirm the removal.



Right-click on parent node in editor view

### Save to Clipboard

To remove but save a copy on the Clipboard, choose Cut. You will not be prompted for confirmation.

## Copy/paste items

### Copy

To **copy** an item, right-click in the editor view and choose **Copy**. The XML snippet will be shown in the Clipboard.

### Paste

To **paste** an item that appears on the Clipboard, right-click in the editor view **on the parent item** and choose **Paste**. Choose an item from the **drop-down list**.

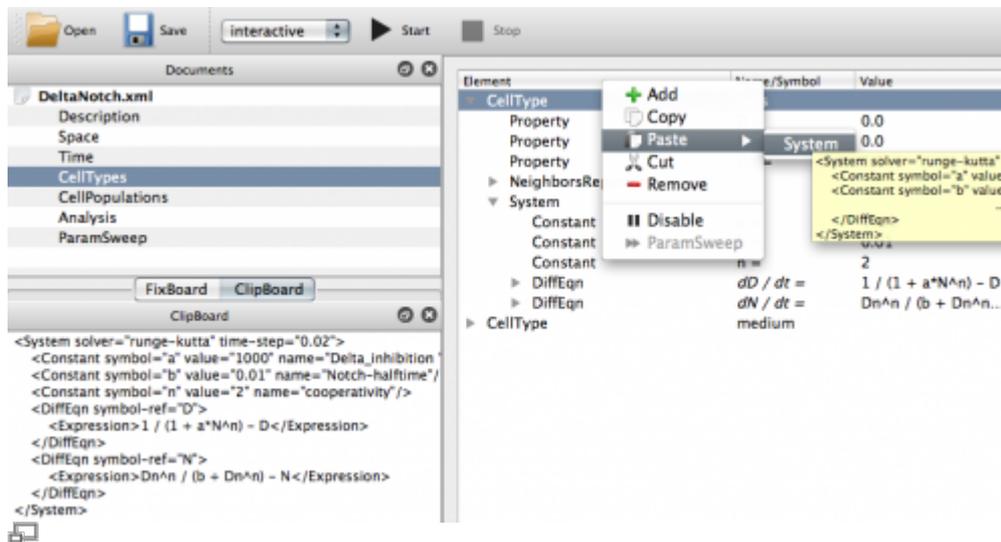
Note that you can copy/paste between different models.

An extract of the XML will be shown as a **tooltip**. This enables you to distinguish items with identical

names.

## Clipboard

Snippets of XML that were copied or cut are shown here. The Clipboard is shared over all models in the Documents view.



## Copy/Paste between models

During model construction, it is often useful to copy/paste items between different models that appear in the Documents view. For instance, to integrate single-scale models into a multi-scale model.

This is possible, because the Clipboard is shared over all models in the Documents view.

## Disable items

### Disable

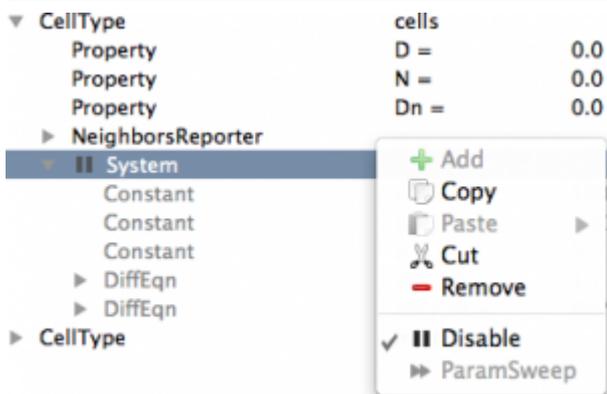
During the model construction or testing process, it is often desirable to temporarily **switch off an item** of the model without removing it from the model.

To **switch off** an item, right-click in the editor view and choose **Disable**. A 'pause' symbol appears before the node, and the item as well as its child nodes are grayed out.

Note that the item is still saved to XML, but is commented out.

### Re-enable

To re-enable, do the same: right-click in the editor view and choose **Disable**.



Switch off a model item by right-click and choose Disable.

## Edit XML model without GUI

### Text editor

The XML files can be opened in any text editor that allow you to manually edit the model.

### Command line tools

More advanced editing of the XML files requires command line tools like [xmlstarlet](#).

For example, to remove all Property items from the CellType called ct1, do:

```
xmlstarlet ed -d "/MorpheusModel/CellTypes/CellType[@name='ct1']/Property"
model_old.xml > model_new.xml
```

## GUI

### Execution mode: "interactive", "local" or "remote"?



Use **interactive** to direct visual output to screen instead of file.

Simulations can be executed in different **job queues** for different tasks.

Local/interactive jobs are started in local job queue that is handled by Morpheus itself. Remote jobs are submitted over a ssh connection to the batch queuing system of the high performance computing resource (e.g. LSF).

### Local / Interactive / Remote

Roughly, local mode is the 'normal' mode for simulation, while interactive mode is for rapid testing.

In interactive mode:

- Visual output (e.g. Gnuplotter) is directed to an on-screen terminal by overriding the specified

terminal.

- Stop current interactive job from toolbar button.

## Remote

Remote mode submits a job to the queueing system on a remote high performance computer.

Remote mode requires password-less ssh authentication (i.e. using "`ssh-copyid`"). Specify username/password details under File → Preferences → Remote.

On first use, Morpheus copies a proxy script to the remote computer through which Morpheus communicates with the job scheduling system. Morpheus is shipped with a proxy script for [LSF](#), but this can easily be adapted to other scheduling systems.

| Job queue   | Purpose                 | Behavior   |
|-------------|-------------------------|--|
| Local       | Normal processing       |  |
| Remote      | Remote batch processing | Submit job to remote queueing system (e.g. LSF) on high performance computing resource.<br><b>Note:</b> Feature not yet available in public version                        |
| Interactive | Testing mode            | Start/Stop simulations from toolbar buttons.<br>Directs visual output to on-screen terminal.<br>Overrides Gnuplotter terminal to wxt (Linux), aqua (Mac) or win (Windows). |

## FixBoard

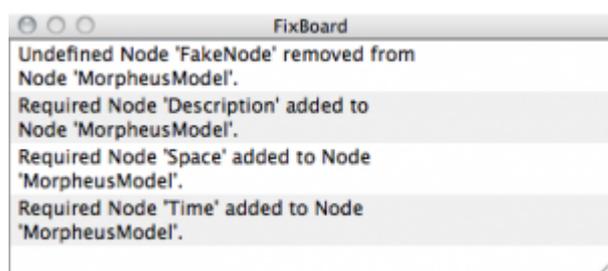
### FixBoard

When you open a outdated or broken XML model, Morpheus will try to automagically correct and update the model. For example, Morpheus creates required elements that are missing and removes obsolete elements.

The changes that Morpheus made are shown on the Fixboard. **You are strongly advised to review those changes.**

As an example, the following message will appear in the FixBoard when we invalidate the [minimal model](#) by removing the Description, Space and Time elements and replace them with an fictitious FakeNode node:

```
<?xml version='1.0' encoding='UTF-8'?>
<MorpheusModel version="1">
  <FakeNode/>
</MorpheusModel>
```





The FixBoard shows the automatic changes made in a broken or outdated model for review.

Note that this is a feature of graphical user interface. The command line interface morpheus cannot correct outdated or broken models supplied as command line arguments.

## JobQueue (job archive)

### JobQueue

This panel has multiple functions:

- Overview of pending, running and terminated jobs
- Archive of simulation models
- Sorting simulation jobs and sweeps
- Access to simulation result browser
- Stop and remove jobs and results

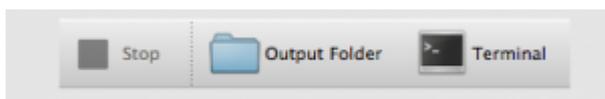
### Result browser

#### Morpheus results browser

Simulation results can be shown by clicking the job in the JobQueue. This opens a file browser within Morpheus showing the Output Folder and the Output Text.

#### File browser and terminal

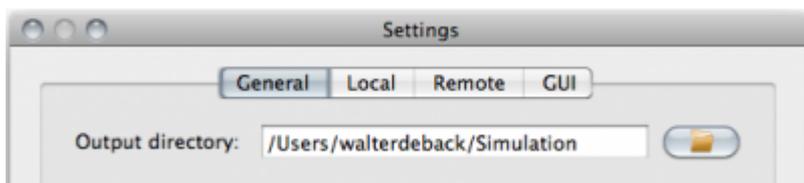
The buttons above the result browser can be used to open the Output Folder your system-wide file browser or open in a Terminal.



Use the buttons to open Output Folder in your file browser or in terminal.

#### Change results folder

To change the folder where results are stored, check the Settings.



The folder where results are stored can be changed in File-Settings.

#### Reset JobQueue archive

The information in the JobQueue is stored in using a SQLite database. This database is named morpheus.db.sqlite and stored in the OS-specific folder for Application Data.

Remove or rename the file `morpheus.db.sqlite` to reset the job archive. Note that this does not remove the simulation results themselves.

## Checkpointing (simulation snapshots)

### Checkpointing

Storing snapshots of the simulation state during execution is called [checkpointing](#).

This allows the user to e.g.:

- Restore a simulation
- Continue a simulation under different conditions
- Use the end-state of a simulation as initial condition of a new simulation

### Enable checkpointing

Checkpointing is switched off by default.

To enable checkpointing, add the item `Time → SaveInterval`.

To set the interval, set the `Time → SaveInterval → value`.

Special cases:

- `value = -1`: Disable checkpointing
- `value = 0`: Store state only at start and end
- `value > 0`: Store state at specified time interval

### File format

Snapshots are saved in a compressed XML format with the filename `[Title][Time].xml.gz`.

### Open saved models

Snapshot files `[Title][Time].xml.gz` can be opened by double-clicking on them in the GUI.

From the command line, first unzip the file and then run `morpheus [Title][Time].xml`

### Limitations

The snapshots store the complete simulation state. However, the values of **PDE Layers are not stored**.

This is excluded because of (1) the large storage requirements and (2) the required time to write to text file. (In the future, separate binary files will be written for PDE Layers which can be stored and written more efficiently, but are more difficult to do in a platform independent fashion.)

### Restore parameter sweeps

Parameter sweeps can also be restored. This restores the parameters and value ranges specified for a particular model.

This feature requires an opened model that has the same parameters.

## Settings

### Multithreading / Concurrent jobs

1. Number of threads: Used to set number of openMP threads for (in-job parallelization)
2. Concurrent jobs: number of jobs executed in parallel (between-job parallelization)

### Gnuplot path

By default, Morpheus uses the first GnuPlot executable it can find in the PATH environmental variable. Optionally, you can overrule this path.

### Graphical User Interface

To use a specific GnuPlot version, specify you gnuplot executable under File → Settings → Local → Gnuplot executable.

### Command Line Interface

To specify a gnuplot executable from the command line, you can use the `gnuplot -part` option as command line argument:

```
morpheus -gnuplot-path [File]
```

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